Molecular Foundry User Policies and Definitions

1. Guiding principles

The User Policy at the Molecular Foundry provides a framework for establishing a congenial, collaborative environment where scientifically and culturally diverse researchers can work together in pursuit of the new scientific opportunities presented by this innovative facility.

As a national user facility, access to the Molecular Foundry and its facilities is accessible free of charge to all qualified researchers via a proposal review process. All proposals for research to be conducted at the Molecular Foundry are evaluated by an external panel of subject-matter experts.

2. Safety

Safety is critical for all research conducted at the Molecular Foundry. Users are expected to know and follow all safety requirements. Customized training is provided to all researchers visiting the facility.

Environmental Health and Safety (EHS) training. Users are informed of all necessary training and/or special preparation required to ensure that the project meets LBNL safety standards. Most commonly required EHS training courses are available online. This institutional training is typically supplemented by personalized on-the-job safety training provided by Foundry scientists and technicians. Before work can be authorized, safety training must be completed and any controls specific to the user's project must be implemented. Users must seek further training before using any equipment or technique with which they are not sufficiently familiar to ensure that the risk of damage is minimized. Users who will be onsite for seven days or less and who will be working under the direct supervision of Foundry staff are exempt from formal course requirements, but must be familiar with all relevant EHS requirements.

Working alone. Due to potential hazards in Foundry laboratories, many operations are not permitted when working alone in laboratories outside of normal business hours or under unusual circumstances. All users must read and abide by our Working-Alone Policy.

3. Costs

Access to the Molecular Foundry is free of charge for approved, non-proprietary research; the vast majority of projects fall into this category. Onsite users bear their own living, local transportation and travel costs. A user proposal must estimate the amount of project support, including the reagents/supplies that would be needed from the Molecular Foundry. In the rare circumstance where a user's project requires consumable items above and beyond what is customary, he/she will be asked to establish a charge account to handle these more costly incidentals.

Proprietary projects pay a "full cost recovery" rate during the period when the project is active.

4. **50/50 staff time model**

   All Foundry scientific staff split their time evenly between supporting users and developing their internal research programs, in accordance with our "50/50" model. This model incentivizes staff to develop capabilities that are relevant to the user community and keeps them fully engaged in pursuit of problems they are passionate about.

5. **User proposal types**

   Each proposal type may last up to one year, which begins on the project's first day of work. Research that requires addition time at the Molecular Foundry will require additional successful proposal applications.

   a. **Standard proposals**

      Standard proposals provide the most common pathway to Foundry capabilities and are evaluated during the two calls for proposals each year. A standard proposal may require the use of a single Foundry facility or several. Multi-facility proposals are encouraged and can result in more favorable proposal ratings since they make the best use of the Foundry's unique, multidisciplinary capabilities.

      All proposals undergo an in-depth internal and external peer review. This review consists of internal administrative and scientific feasibility review, EHS review, and evaluation by an external Proposal Review Board composed of experts in the field of proposed study. Notification of proposal acceptance or rejection occurs within 10 weeks of the submission deadline.

      An approved User Agreement between all institutions identified in the proposal and LBNL is required, in addition to an EHS review.

   b. **Rapid access proposals**

      Rapid Access proposals provide an accelerated pathway to Foundry capabilities outside of the biannual proposal calls. This mechanism should be used exclusively for time-sensitive research with high potential impact, and with direct relevance to the Foundry's research themes. The Foundry User Office (foundry-useroffice@lbl.gov) can offer preliminary feedback on whether Rapid Access is appropriate for a given proposal. Rapid Access proposals can be submitted at any time and undergo an accelerated scientific peer review.

   c. **Sample-only proposals**

      Sample-only proposals are requests for materials already available or regularly synthesized at the Foundry, such as routinely generated peptoids or quantum dots. These projects receive accelerated review for feasibility and merit by the Foundry Directorate. Sample-only proposals are accepted and evaluated continuously throughout the year. A Materials Transfer Agreement (MTA)or, in the case of a biological-based sample request, a Uniform Biological Material Transfer Request (UBMTA), rather than the normal User Agreement is required to be executed prior to project activation and shipment of samples.

   d. **Instrument-only proposals**

      Instrument-only proposals are for projects that require limited access to one or two Foundry instruments, excluding NCEM instruments. These projects receive accelerated review for feasibility and merit by the Foundry Directorate and by

external subject-matter experts, as needed. A formal User Agreement is still required with each institution named in these proposals, as well as EHS evaluation and approval. Instrument-only proposals are accepted and evaluated continuously throughout the year.

e. Proprietary proposals

A proprietary proposal is like a standard proposal, but with the intent to withhold research results from publication for up to 5 years. Although the proposed work may be proprietary, sufficient information must be included in the proposal to permit evaluation of its scientific merit.

6. Proposal questions and evaluation criteria

a. Scientific Significance and Impact (30 points)

Proposal question: Describe the scientific or technological motivation, long term goals, and significance/impact of this project in the context of the field of study. (300 – 400 words)

Review criteria: To what extent is the proposed research expected to significantly advance the scientific or technological field? How likely is the proposed work to produce impactful publications?

b. Project Plan (10 points)

Proposal question: Describe your project plan. Clearly outline the scope of work you intend to do at the Foundry within the project term. Be explicit about which aspects will be done at your home institution. (300 – 400 words)

Review criteria: Is the experimental plan achievable at the Foundry within the proposed project term (not to exceed one year)? How will the results obtained at the Foundry complement and propel further follow-up research at the user's home institution?

c. Need for the Molecular Foundry (10 points)

Proposal question: Describe your need for specific advanced capabilities and expertise at the Foundry. If applicable, highlight any interdisciplinary aspects of the project that may require the unique combinations of capabilities of the Foundry. (300 – 400 words)

Review criteria: How well justified are the Foundry resources requested? To what extent will the proposed work take advantage of the unique capabilities or combinations of capabilities/expertise either within a single facility, or across the Foundry as a whole?

d. Relevant Experience (10 points)

Proposal question: Describe the experience and accomplishments of each researcher in relation to the proposed work. (100 words per researcher)

Review criteria: How do the users' track records of innovative, technically demanding research inform the likelihood of success of the proposed project? Are the users adequately prepared for efficient use of limited Foundry resources?

e. Support Facility Justification

Proposal question: If applicable, describe the importance of the requested support facility or facilities toward accomplishing the project goals, highlighting specific points of complementarity. (100 words per facility)

Review criteria: To what extent is use of the proposed support facility expected to benefit the primary goals of the project? How well is this additional facility resource request justified?

No score given. Comments made by support Facility Director.

f. Molecular Foundry Utilization Timeline

Proposal question: Describe the expected timeline of the project, including an estimate of the number and frequency of facility usage visits. (300 – 400 words)

Review criteria: Consider the relative amount of both personnel and instrument resources effectively requested by this proposal. Will the proposal have a low, medium, or high impact on the typical operation of this facility?

Effort rating of low/med/high and comments made by lead Facility Director.

7. Proposal Review Board (PRB) and review process

The Molecular Foundry's PRB is an external body (i.e. non-Molecular Foundry Staff) of subject-matter experts from various fields of nanoscience research, technology and industry. PRB members are nominated by the Molecular Foundry's Facility Directors and serve by concurrence of the User Program Director. Members typically serve a term of at least two years.

The PRB meets twice a year to review standard proposals submitted to the Molecular Foundry. Each proposal is assessed in four specific areas: scientific merit, project plan, need for the Molecular Foundry, and relevant experience. The Foundry accepts as many of the top-rated proposals as capacity allows. PRB members who are directly involved in a proposal or conflicted in any other way do not participate in the discussion or scoring of that proposal.

The evaluation criteria used in the peer review (listed above) are based on criteria recommended by the International Union of Pure and Applied Physics for major user facilities: scientific merit; technical feasibility; impact on field of inquiry; and capabilities of the investigator(s).

8. User agreements with Berkeley Lab

All Foundry users must execute a User Agreement with Berkeley Lab. This agreement, between the user's institution and Berkeley Lab, forms the contractual basis covering the distribution of intellectual property rights. With respect to patent protection, Foundry users may, in most cases, receive advance rights to any inventions or proprietary data developed under the user agreement whereby the user has the option to take title to such inventions. The technical data may be deemed proprietary if the user pays full cost for the use of the facility, as described below. The U.S. Government reserves certain rights to intellectual property and those rights are outlined in the agreements as negotiated between the parties.

Non-Proprietary Research

- Non-Proprietary User Agreement (NPUA) – Collaborative & Non-Collaborative (Preferred)
    - All incoming data and data generated is non-proprietary
    - All results can be freely published/shared
    - Users alone (non-collaborative) or users & LBNL (collaborative) are performing work on the project

- Cost to users is $0 unless the project requires significant LBNL effort or expenses above and beyond an ordinary user project

- Work for Others (WFO) – Collaborative & Non-Collaborative
  - LBNL is performing research for user above and beyond ordinary user project
  - (can be used in conjunction with NPUA or as a stand-alone Agreement)
  - Incoming user data may be proprietary
  - LBNL data generated is non-proprietary and can be freely published/shared
  - LBNL is performing research work on the project
  - User pays full costs of LBNL work
- Cooperative Research and Development Agreement (Standard) – Collaborative
  - Incoming user data may be proprietary
  - User may keep their generated research results private (no expectation to publish)
  - For a standard CRADA, LBNL data generated is non-proprietary and can be freely published/shared
  - User & LBNL are collaboratively performing research on the project
  - User (or another sponsor) pays full cost of LBNL work

Proprietary Research

- Proprietary User Agreement (PUA) – Non-Collaborative (users only performing research)
  - Incoming user data may be proprietary
  - User may keep their generated research results private
  - User is performing research on the project
  - LBNL technical assistance only is being utilized (LBNL will not generate data)
  - User pays full costs of use of facility & LBNL assistance
- Cooperative Research and Development Agreement (Non-standard)

  For Use in exceptional circumstances only. Requires both Foundry Director and LBNL Lab Director approval. LBNL Lab Director approval is required for any LBNL researcher to collaborate on research that requires results to be kept proprietary and/or for publication of results to be pre-approved or withheld by the user team
  - Incoming data may be proprietary
  - User may keep their generated research results private
  - User may request to keep LBNL-generated research results private (no expectation to publish)
  - User & LBNL are performing research on the project
  - User pays full cost of use of facility and LBNL work

9. Access to other user facilities at LBNL

The Molecular Foundry is immersed in a vibrant research environment at LBNL and the surrounding area. In addition to the Foundry, LBNL is home to three other national user facilities. Two of these facilities, listed below, have special arrangements with the Foundry. More information about all the facilities can be found on the LBNL website.

Advanced Light Source (ALS). Access to ALS instruments can be requested during the Molecular Foundry's proposal submission process and is managed by the ALS User Programs Office and appropriate beamline scientist(s). Beam time for Foundry users has

been arranged through a memorandum of understanding (MOU) and allows Foundry users to request three shifts of beam time per proposal. ALS access for approved Foundry projects is contingent on availability.

National Energy Research Scientific Computing Center (NERSC). Access to NERSC is requested via the Molecular Foundry proposal creation forms and is managed by the Theory Facility Director, who each year receives an allocation of NERSC resources for Molecular Foundry user needs.

10. Final project report

Users are required to submit a final project report within 30 days of completion of their project. Proposals submitted by former users who have not submitted their final project reports will not be accepted. A discussion of the project progress and results along with a list of the resulting publications or patents is required.

11. Publications and acknowledgement

Reprints of publications resulting from work done at the Foundry must be sent to the Foundry User Office at foundry-useroffice@lbl.gov. The Foundry compiles a list of all of these publications, and makes it available in various publications and reports.

The following acknowledgment must be used when referencing work performed at the Molecular Foundry:

> *Work at the Molecular Foundry was supported by the Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.*

For more complex funding combinations, refer to the Materials Sciences Division website.

It is expected that all user project results of sufficient scientific merit will be prepared for publication and submitted to a journal. Any Foundry scientist who made significant contributions should be included as an author and will expect to review the paper before its submission to a journal.

12. User feedback and end-of-project survey

The User Office welcomes feedback from users to help improve user services and the Foundry website. To share feedback, users are encouraged to either email the User Office at foundry-useroffice@lbl.gov, contact members of staff directly, or visit the User Office on the third floor of the Foundry.

As part of an annual DOE reporting process, the Molecular Foundry and other DOE facilities are required to ask users to take part in a survey to provide demographic information and feedback to the Office of Basic Energy Science (BES). Users will receive an email invitation to complete the survey after their project ends, and are asked to respond in order to improve user services at the Molecular Foundry.

13. Users' Executive Committee (UEC)

The UEC serves as an advocacy group for users at the Molecular Foundry and its user community, and ensures good communication between the Foundry user community and Foundry management. The UEC is also responsible for organizing the scientific content of the Annual Users' Meeting.

All users are encouraged to interact with the UEC and get involved. More information on the UEC can be found on the UEC website.

14. Scientific Advisory Board (SAB)

The SAB comprises distinguished scientists from the numerous scientific disciplines that bear on nanoscience and represent academic, industrial and government laboratories. The SAB meets annually, often in conjunction with the Annual User Meeting, to review the Foundry's scientific programs and operating procedures. Feedback from the SAB has guided the development of Foundry-wide research themes, equipment and staffing priorities, and has identified areas of opportunity for user projects.

15. Conflict resolution

Researchers are encouraged to think beyond the science, and to reflect genuinely on the ethical standards of their activities and whether engaging in those activities could lead to a potential or real conflict of interest within the community. Facility Directors are available to mentor individuals in these instances to preempt conflict, and the User Office Director is available to assist users in conflict resolution.

The Molecular Foundry has a formal grievance mechanism to resolve conflicts that arise among the community of users and staff. Parties seeking redress or resolution of a conflict can petition the Foundry Director, who will, if warranted, appoint an ad hoc committee to review the matter under dispute. The committee, composed of representatives from the Scientific Advisory Board or Foundry community, will advise the Director on the fair resolution of the dispute.

16. Data management

All proposals submitted to the Molecular Foundry should include written acknowledgment of, and agreement with, the Molecular Foundry's Data Management Statement, as given here.

If you propose to use facilities or resources at the Molecular Foundry, please be aware of the following information, either for inclusion in your Molecular Foundry User Proposal or an associated request for DOE funds leveraging Molecular Foundry resources, which must contain a Data Management Plan.

Currently, all Molecular Foundry Users are responsible for their own Data Management associated with their approved and active User Projects. If you have questions regarding our Data Management policy, you are encouraged to contact the User Office at foundry-useroffice@lbl.gov and/or your User Project's Assigned Staff Scientist.

Resources: Users are free to use personal mass storage devices, laptops, tablets, cell phones and lab notebooks for data storage and eventual transfer to their home institution. Foundry facility-based access to cloud storage and backup is available to Users, in some cases for a nominal fee (e.g., Google Drive, Dropbox, Carbonite). Data stored in the cloud can be shared by standard means. For user work performed on instruments within our facilities, Users must transfer data first to a file server or local storage device or else request the transfer via Foundry staff. Software for data analysis is available on local computer desktops in-house; users are free to utilize their own provided resources. Computational resources exist and follow LBNL standard practice for temporary storage of User data files backup for the duration of their projects.

Practices: For specific instruments in most facilities, staff-originated data back-ups occur regularly; files transferred to institutional storage (file servers) are backed up daily, but Users are generally responsible for their own data preservation. User data is only

preserved during the project lifetime and no guarantees are provided once the project ends, although some facilities maintain data long term/indefinitely. Access to data is associated with the status of a User Project and once terminated data access and preservation rights may be lost. All data generated on collaborative non-proprietary user projects funded by DOE and referenced, utilized or included in subsequent publications is expected to be made public upon request.

Policy: All data generated on a Foundry collaborative project is jointly owned by both users and LBNL unless otherwise defined in executed User Agreement documents. Data generated on non-collaborative projects may be owned exclusively by the Users. No restrictions on file formats due to heterogeneity currently exist.